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AUTHORS: Burovoy, I. A., D'yachko, A. G.

TITLE: Mathematical simulators for fluidized bed apparatus to study thermochemical processes

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TEXT: Equations for the rates of adsorption, desorption, and reaction are derived for the heterogeneous chemical reaction in a fluidized bed: $a_1A_1 + a_2A_2 = a_3A_3 + a_4A_4$, where A_1 is the solid, and A_2 is the gaseous initial substance, A_3 is the solid and A_4 the gaseous reaction product, and a_1, a_2, a_3, and a_4 are the stoichiometric coefficients.

$v_a = C^F_{A_2} \sum_{i=1}^{n} K^o_{ai} \cdot \Theta_{oj} \cdot \exp\left[-(E^o_{ai} + \sum_{(j)} \eta_{A_j} \Theta_{A_j i})/RT\right]$ (11) holds for the adsorption rate of A_2 with respect to unit surface, $C^F_{A_2}$ is the

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concentration of A_2 on the active surface (m^{-3}); K^o_{ai} is a factor having the dimension m^3/sec; E^o_{ai} is the activation energy of the free surface; $\eta_{A_j} = \alpha_j b_{A_j} C_{s\infty}$, where α is the change of energy due to adsorption, b is a coefficient, and $C_{s\infty}$ is the concentration of the adsorption centers per unit of surface; $\Theta A_j i = C^s_{A_j i}/C_{s\infty}$ is the degree of surface occupation by the substance $A_j i$, with $C^s_{A_j i}$ being the surface concentration of $A_j i$.

$v_{di} = \sum_{i=1}^{n} K^o_{di} \cdot \Theta_{A_2 i} \cdot \exp\left[-(E^o_{di} - \sum_{(j)} \eta'_{A_j} \Theta_{A_j i})/RT\right]$ (17) holds for the desorption rate of A_2 per unit surface. $v_r = \sum_{i=1}^{n} K^o_{ri} \cdot \Theta_{A_2 i} \cdot \exp(-E_{ri}/RT)$ (22) holds for the total rate of the chemical reaction. $d\Theta_{A_2}/dt = v_a - v_d - v_r$, wherein the values from equations (11), (17), and (22) are to be substituted, holds for the material balance. For the substance A_4, the

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equations for adsorption, desorption, and material balance are set up in the same way. The functional diagram of the simulator (Fig. 1) correctly reproduces the course of the heterogeneous thermochemical processes, when the adsorption of A_2, the desorption of the reaction product, or the chemical reaction on the active surface are the limiting stages. There are 2 figures.

Fig. 1: Functional diagram of the mathematical simulator for adsorption, desorption, and surface reaction of a heterogeneous process. Legend: α = a = adsorption; ϑ = d = desorption; ρ = r = reaction.

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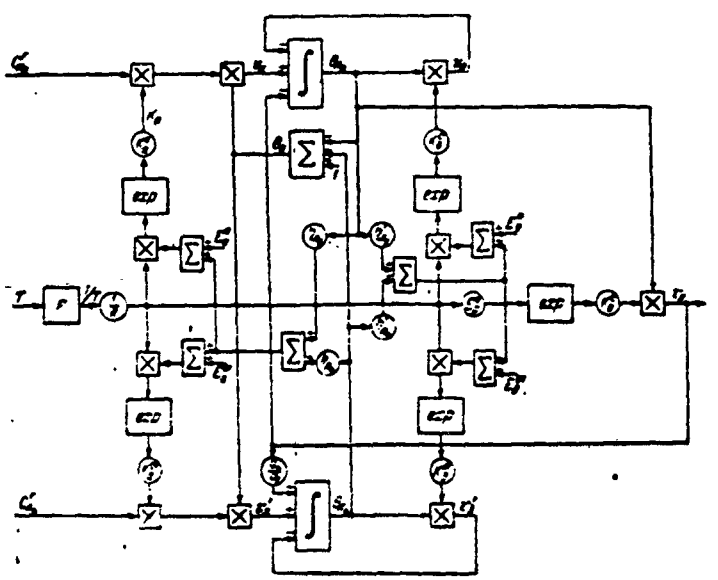

Fig. 1

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